Artificial Intelligence hubs for Scientific and Engineering Research

[Link to funding opportunity]

Summary of Successful Outline Proposals (Ordered by grant number)

Grant No.	PI	Title
EP/Y007069/1	Professor Matthew Gaunt	AI for Molecule Making
EP/Y00714X/1	Professor Omer Rana	Hub on "Edge AI for Sensing & Optimisation"
EP/Y007506/1	Professor Craig Butts	AI Hub for Digital Chemistry - Trustworthy Discovery & Insight
EP/Y007522/1	Professor Jim Al-Khalili	AI Meta-Physics: Fusion of Quantum AI and Quantum Topological Materials (AIM)
EP/Y007573/1	Professor Adham Hashibon	Novel AI for Accelerated Materials Design & Discovery (AI4MD)
EP/Y007611/1	Professor Andrew Cooper	AI for Chemistry: AIchemy
EP/Y007700/1	Professor Barbara Shollock	Artificial Intelligence for a Changing Economy - enabling efficient, effective and sustainable products (AICE)
EP/Y007719/1	Professor Konstantinos Tsavdaridis	AI for Megacity Building Lifecycle Management Hub
EP/Y007786/1	Professor Themis Prodromakis	AI for Productive Research & Innovation in eLectronics (APRIL)
EP/Y007808/1	Professor Leroy Cronin	Open Network for Artificial Chemical Intelligence & Discovery Hub (ON-ACID)
EP/Y007875/1	Professor Samuel Kaski	ML4Science: The AI Hub on Machine Learning for Science
EP/Y00793X/1	Professor Praminda Caleb-Solly	The National Hub for EMBodiED AI in Healthcare (EMBED-AI)

Grant Reference Number: EP/Y007069/1

Title: AI for Molecule Making

Team:

- Professor Matthew Gaunt, University of Cambridge (PI)
- Dr Jose Miguel Hernandez Lobato, University of Cambridge
- Professor Fernanda Duarte, University of Oxford
- Professor Jeremy Frey, University of Southampton
- Professor Jonathan Hirst, University of Nottingham
- Professor Ross King, University of Cambridge

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Brief description of proposed work:

Machine Learning (ML) and Artificial Intelligence (AI) are central to the future of chemistry and will enhance our ability to design & synthesize the molecules of function that will impact tomorrow's society. These molecules include the medicines we use to treat disease, the agrochemicals we need to provide food security, the basic components of advanced materials that drive technology and the commodity chemicals that support the everyday life that we take for granted. While traditional approaches have proven capable of supplying society with these essential molecules, the current molecular discovery and development process is under severe pressure. In particular, the continuing increase in molecular complexity, environmental constraints on how we make molecules and increasingly aggressive business-driven timelines for delivery mean that we often miss out on essential products that we will need in the future.

Our Hub on 'AI for Molecule Making' will address these challenges by creating new ML & AI approaches that will revolutionize molecule synthesis, eliminating risk factors that have plagued this process for years. By analysing vast amounts of chemical data, these methods will be able to predict what is the best molecule to make, how to make it efficiently and design a process that automates its synthesis. Furthermore, these computational approaches will also alert us to opportunities in chemistry and synthesis that the human mind may have missed, which means that instead of having to solve the routine tasks that would now be potentially automated, the human mind can be turned to thinking about how to explore these new areas of chemical space uncovered by AI.

This type of approach would represent a paradigm shift in molecule synthesis and can only have a positive impact on our future. Alongside the advances that ML and AI will instil on chemistry and synthesis, the new computational models will also feedback into the general ML & AI research scene, where it has been repeatedly shown that advances in one domain can have substantial impact when applied elsewhere.

The Hub will bring together AI/ML specialists with leading computational & synthetic chemists to create a dynamic environment for AI-driven synthesis. The resulting synergies will provide the foundations for new interdisciplinary research in ML & AI, biomedical science, agroscience, advanced materials & commodity chemicals by accelerating the design & synthesis of new molecules of function. Importantly, this Hub will help create a new inter-disciplinary research community of AI researchers and chemists working together. This community will be placed in a unique position to solve the molecule synthesis problems that affect our present and future society.

Grant Reference Number: EP/Y00714X/1

Title: Hub on "Edge AI for Sensing & Optimisation"

Team:

- Professor Omer Rana, Cardiff University (PI)
- Professor Lee Chapman, University of Birmingham
- Professor Luc Moreau, King's College London
- Professor Muhammad Imran, University of Glasgow
- Professor Philip James, Newcastle University
- Professor Theodoros Tryfonas, University of Bristol

Brief description of proposed work:

Urban and rural observatories enable data collection about our use of transport systems, people movement/ flows, energy and environmental resources and more. Significant investments have been made in such observatories to create scientific and engineering applications that can utilise common sets of data collection, management and visualisation services. Applications can include: (i) precision farming and managing emissions from farms; (ii) investigating air quality in cities and urban environments; (iii) calculating footfall in particular parts of the city to inform city planning and high streets, (iv) planning "corridors" for electric (and potentially hydrogen) vehicles to ensure availability of suitable charging (re-fuel) locations etc. Supporting AI and Machine Learning (ML) in such applications can impact a variety of different application areas that make use of data from urban and rural observatory platforms.

Utilising AI/ML algorithms to analyse data from urban and rural environments can also be used to predict additional services that may be of interest to citizens, and conversely how existing infrastructure (e.g. for transport, energy) is utilised. Ensuring that this can be undertaken ethically and whilst preserving the privacy of citizens also remains a challenge, considered across a number of privacy legislation (Data Protect Act, GDPR compliance) and policy requirements.

The novelty of this AI Hub is the use of edge computing environments (systems and services) to create a new class of AI algorithms and applications for urban/ rural sensing. Edge computing enables use of computational capacity that is closer to the user, often in-proximity to the data generation or actuation source. Significant recent investments in AI have focused on improving the size and complexity of learned models, requiring the use of large-scale computational resources managed at a data center to develop such models. Edge computing instead focuses on utilising AI models that can be hosted on resources that have (comparatively) lower computational and storage resources. As investment in rural and urban sensing increases, e.g. through the use of new sensing technologies and mobile apps that can generate crowd sourced data, so does the computational capacity of edge environments. Edge-AI, the focus of this Hub, is not to replace large scale models hosted at a data center, but to complement and extend these with capacity available within edge environments -- providing a number of benefits: (i) better energy usage profiles; (ii) improved data privacy; (iii) efficient use of user owned resources, especially for applications that have strict latency/ real-time requirements.

An intelligent edge environment, coupled with capacity at a data center, can be transformative for how we use and develop the next generation of urban and rural observatories. Similarly, understanding how constraints (computational, data storage, and network connectivity) within an edge environment can change how we design, develop and deploy AI algorithms, and modify AI models that have been trained at data center for use on resource constrained devices, will be key challenges shaping the activities of this Hub.

Grant Reference Number: EP/Y007506/1

Title: AI Hub for Digital Chemistry - Trustworthy Discovery & Insight

Team:

- Professor Craig Butts, University of Bristol (PI)
- Dr Charlotte Willans, University of Leeds
- Professor George Panoutsos, University of Sheffield
- Professor Ian Nabney, University of Bristol
- Professor Mahesan Niranjan, University of Southampton
- Professor Richard Bourne, University of Leeds

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Brief description of proposed work:

Many aspects of our daily lives are reliant on the power of chemistry to produce compounds and materials quickly, cleanly and with complete control over their properties. This underpins our healthcare system, where pharmaceuticals can be used to treat illness and prolong life, it enables a pivot towards a net-zero economy through better energy storage materials, and manufacturers to supply better buildings and transport, as well as protecting food and water supplies.

This Hub will bring together chemists and artificial intelligence specialists, across academia and industry to try and answer an apparently simple question - how can we make artificial intelligence tools that can build on and enhance the scientific skills and expertise of modern chemists. With such tools in hand, we will enable the chemists of the future (digital chemists), skilled in machine learning data science and automated chemical science, who will be the driving force behind the UK's world leadership in chemical and pharmaceutical research and manufacturing.

The challenges of chemical reactions are so complex however, that even cutting-edge algorithms struggle to scratch the surface. For example, there are roughly a million billion billion billion possible molecules that might be effective medicines - so how can we begin to get a computer to work out which one is the best and how to make it quickly and sustainably? Existing AI tools for chemists generally focus on optimising single processes and understanding single chemical systems, but the future of this field needs generalisable tools that can be applied to designing and making any of those molecules, as well as providing us scientific insight into what is going on during those processes. We also need to build in appropriate controls to prevent abuse of these systems and develop approaches that can decide what the next round of experiments will be, so that automated (robotic) systems can find better solutions more quickly, with minimal intervention.

To create such tools this Hub will deliver two core things: the most modern, indeed new, AI approaches combined with the highest quality, cutting edge and reproducible chemistry data. We need to bring together communities of experts in chemistry, computing, AI and mathematics to develop new monitoring equipment, integrate and interpret data from a variety of sources and ensuring the AI is trustworthy by rigorous validation and protocols. We will bring these to bear on the challenges of chemical reactions which are important for society and sustainability as well as UK prosperity, for example replacing expensive and unsustainable precious metal catalysts (palladium, platinum) with cheap and sustainable earth-abundant metals (iron, copper).

Grant Reference Number: EP/Y007522/1

Title: AI Meta-Physics: Fusion of Quantum AI and Quantum Topological Materials (AIM)

Team:

- Professor Jim Al-Khalili, University of Surrey (PI)
- Dr Alexander Balanov, Loughborough University
- Dr Marian Florescu, University of Surrey
- Dr Sergey Kafanov, Lancaster University
- Dr Uraz Turker, Lancaster University
- Professor Amalia Patane, University of Nottingham
- Professor Ivan Tyukin, King's College London
- Professor Kelly Morrison, Loughborough University
- Professor Plamen Angelov, Lancaster University
- Professor Qiang Ni, Lancaster University
- Professor Sergei Novikov, University of Nottingham
- Professor Sergey Saveliev, Loughborough University
- Professor Wenwu Wang, University of Surrey
- Professor Yuri Pashkin, Lancaster University

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Brief description of proposed work:

A well-known physics joke goes like this: two-body problems can be solved exactly in Newtonian mechanics, and single-body-in-a-vacuum problems can be solved exactly in non-relativistic quantum mechanics. Still, in quantum field theory, we cannot even solve the vacuum problem since we cannot define the vacuum reliably. Therefore, physics is useless. This light-hearted statement cannot obscure that physics has been astonishingly successful in describing our world, and the technologies being developed based on this understanding continue unabated in the 21st century. Nevertheless, it is undoubtedly true that much of what physics has revealed about reality has been based on phenomenological models involving various approximations and assumptions.

We are then therefore to consider the following fundamental question; might we not be able to make better predictions with more accurate models and simulations? With advances in computing technologies and artificial intelligence we can now task a machine to predict physical reality from a combination of phenomenological knowledge and data instead of solving those imprecise phenomenological equations themselves.

Grant Reference Number: EP/Y007573/1

Title: Novel AI for Accelerated Materials Design & Discovery (AI4MD)

Team:

- Professor Adham Hashibon, University College London (PI)
- Dr Brooks Paige, University College London
- Dr Jeyan Thiyagalingam, STFC - Laboratories
- Dr Stefan Szyniszewski, Durham University
- Professor Ashiq Anjum, University of Leicester
- Professor Jeremy Frey, University of Southampton

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Brief description of proposed work:

AI4MD collates top UK experts in AI, data science, ontology, materials informatics (fusion of materials science and computer science), computer scientists, and materials scientists (both computational, across all scales, and experimental, especially from the field of high throughput formulations and characterisation) to perform a holistic research programme that combines and integrates novel AI, high throughput materials data creation and curation, high throughput computations and experiments/characterisation to achieve a step change in the way novel materials and processes are developed and designed. The main idea is to traverse the Process-Structure-Properties-Performance (PSPP) chain top-down, i.e., from starting from the Properties, use novel AI to solve the multivariable optimisation problem finding the best sets of Properties giving rise to these Performance indicators, then use novel AI to predict the most suitable structures producing such Properties (structure, composition, interfaces, chemistry etc), and eventually use novel AI to predict possible processing routes that result in such a structure.

Eventually, an outer optimisation loop that controls and orchestrates both the high throughput as well inner novel AI loops is trained using novel enforced learning algorithms. Moreover, advanced Uncertainty estimation methods are developed to predict the applicability and accuracy of the predictions.
The project is focused on Li and post Li technologies, hydrogen technology materials , and programmable metamaterials for for novel energy and sustainable materials for environmental applications.
The Hub will be centred around 5 geographical locations, starting from UCL (London) and spreading to Leicester, Durham, Darsebury, and Sauthampton and will expand to cover the entire UK.

Grant Reference Number: EP/Y007611/1

Title: AI for Chemistry: AIchemy

Team:

- Professor Andrew Cooper, University of Liverpool (PI)
- Dr Jacqueline Cole, University of Cambridge
- Professor Jeremy Frey, University of Southampton
- Professor Katie Atkinson, University of Liverpool
- Professor Kim Jelfs, Imperial College London
- Professor Ruth Misener, Imperial College London

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Brief description of proposed work:

Chemistry impacts most areas of our lives, including healthcare, energy production, and the environment. This hub will bring the transformative power of artificial intelligence (AI) to the area of chemistry, and by doing so have a major societal impact. Both AI and chemistry are fast-moving and historically separated research disciplines, and there is huge untapped potential to collaborate at the interface of these two fields. Today, relatively few UK experimental chemists are exploiting AI, and leading examples of AI in chemistry demonstrate the broader missed opportunity; e.g. in efficient reaction optimisation. The use of machine learning methods is more common in computational chemistry, but many examples use off-the-shelf methods. In some AI fields, such as natural language processing, there is also rapidly evolving, leading-edge industrial research, necessitating a cross-sector approach if we are to exploit the cutting edge of this technology.

This hub (AIchemy) will bring together leading researchers in AI and trailblazers at the interface of AI for chemistry, spanning both university and industry. We will exploit unique established facilities and institutes in the four core partner institutions (Universities of Liverpool, Imperial, Cambridge, and Southampton) where cross-discipline working has already been achieved: this includes the Materials Innovation Factory (MIF), the Institute for Digital Molecular Design and Fabrication (DigiFAB), and the I-X Centre for AI in Science. In addition to the 6 listed co-investigators, we have aligned 22 other investigators across the four core institutions, spanning the areas of AI, robotics, and a diverse range of experimental and computational chemistry sub-disciplines. The team also includes unique expertise in robotics and automation (Liverpool & Imperial), natural language processing for chemistry problems (Cambridge) and data curation in the Physical Sciences Data Infrastructure (PSDI, Southampton). This diverse team and associated facilities give us the breadth of expertise and critical mass to become the core of a UK hub for this activity.

AIchemy has three core aims: (i) we will carry out world-leading research at the AI/chemistry interface, building on distinctive UK strengths in this area and developed initially via 6 'Forerunner Projects'; (ii) build an approach for sharing chemistry research data and code in a common format to unite the currently fragmented UK research landscape. A third aim is to broaden the number of AI researchers tackling chemistry problems, and vice versa, through a mixture of pump-priming funding in the hub, bespoke training, access to datasets, and events (e.g., annual AI challenge from hub-generated data). To ensure the long-term health of this discipline, we will also focus resource on projects that are led by early career academics.

The hub will build a UK-wide consortium involving university and industry stakeholders outside of the core partners, including the UK Catalysis Hub, STFC, and a broad set of 26 industry partners across the sectors of AI and chemistry, to be further expanded in the full proposal. The team has an excellent collective track record in industry engagement and knowledge transfer; e.g. MIF collocates 100 industry researchers in a common facility with academics; Chemistry is co-located with IX at Imperial's £2 Bn White City campus, and there are shared spaces to enable 800 scientists and industry partners to work together on common challenges, with tailor-made labs and offices for early stage companies. I-X (established 2021) already has several associated AI start-ups associated (e.g., Deep.Meta, Deep Render, Surreal Vision).

Mirroring the enormous benefits that have been achieved in other science areas, such as structural biology, this hub will transform the UK landscape for the discipline of chemistry, transforming engagement with AI from a relatively niche activity to a core, platform methodology.

Grant Reference Number: EP/Y007700/1

Title: Artificial Intelligence for a Changing Economy - enabling efficient, effective and sustainable products (AICE)

Team:

- Professor Barbara Shollock, King's College London (PI)
- Dr Luciano Batista, Aston University
- Dr Shan Luo, King's College London
- Dr Yee Mey Goh, Loughborough University
- Professor Adele Marshall, Queen's University of Belfast
- Professor Ioan Felician Campean, University of Bradford

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Brief description of proposed work:

Digitalisation has transformed many aspects of products and services. Manufacturing plants are now data-rich, with sensors detecting process deviations and real-time adjustments driving consistency and quality to ever higher standards, logistics have become smarter allowing consumer orders to be rapidly deployed and stock actively managed. These advances have strengthened our economy, made people's lives easier and opened routes to more effective and efficient innovation.

Optimisation of process control and logistics management are sufficient for some industries, such as foundation industries like steel and cement, and for consumer purchasing. However, in those cases where conflicting requirements for new products and systems come together with fast-moving consumer choices such as beauty products and fashion, the situation significantly increases in complexity. As we layer on other requirements such as regulatory and consumer demands for sustainability and ethics in supply chains, production, use and end-of-life, as well as integrating the route to manufacture into the design process, the complexity multiplies. Since all these factors are interrelated, working in this complex requirement space shifts from a traditional linear design-make iteration or the standard systems engineering V-Model of design, test, verify and validate to a complex multi-parameter space of competing problems that need to be addressed concurrently. AI brings the ability to advance fundamental research in model-based systems engineering by developing frameworks to make decisions and interferences for handling these complex tasks and systems.

In AICE, we will address the complexities of consumer preferences, perceived quality, product design, manufacturing and sustainability and ethical requirements by developing and applying new AI methods and tools to exploit the data-rich complex subsystems that comprise the product lifecycle and supply chains. To achieve this, we will bring mathematical and computational approaches together with the parameters from product design, system requirements and manufacturing to accelerate and optimise decision making. To facilitate interaction for all users, we will develop visualisation tools for quick understanding. We will explore the use of generative AI for co-creation of new products, while considering intellectual property issues that come with this approach.

Grant Reference Number: EP/Y007719/1

Title: AI for Megacity Building Lifecycle Management Hub

Team:

- Professor Konstantinos Tsavdaridis, City, University of London (PI)
- Dr Eduardo Alonso, City, University of London
- Dr Jennifer Schooling, University of Cambridge
- Professor John Ahmet Erkoyuncu, Cranfield University
- Professor Leroy Gardner, Imperial College London

Brief description of proposed work:

The building sector in the UK is responsible for 49% of annual carbon emissions, and over the next 40 years 230 billion square meters of new construction are expected around the world. This evidence, amid the current climate emergency, is calling for immediate action from the construction and civil engineering community to first enhance the performance and value of existing infrastructure and second, to build new only when necessary and driven by more efficient practices through-life.

The disaggregation of the building sector greenhouse emissions in the UK shows that operational carbon emission of the existing building stock is responsible for 80% of the annual total, and only 20% is due to the embodied carbon of new construction. This disparity is even more apparent from an economic point of view, for the construction of new assets increases the total value of UK infrastructure by just 0.5% a year. This is consistent with the evidence that only 1-2% of total building stock each year is newly built in the UK.

This evidence, amid the current climate emergency, is calling for immediate action from the construction and civil engineering community to first enhance the performance and value of existing infrastructure and second, to build new only when necessary and driven by more efficient practices through-life. However, this is a more complex problem, where even before environmental and economic outcomes, people should be at the centre of the raison d'etre of civil infrastructure. This 'people's perspective' becomes more evident if population growth and urbanisation evidence are contemplated. As urban centres grow, the interconnection of infrastructure expands effectively producing a system-of-systems, that should be reflected in the way the infrastructure industry runs. This requires both adaptations of existing AI techniques and the development of solutions for the specific identified needs.

This Hub aims to use existing and develop new tailored AI tools for building lifecycle management through an Evolving Digital Twin (EDT) with sustainability as a main driver. The ambition of an EDT to achieve greener asset through-life management can only be tackled by joining efforts in a Research Hub, and only developed in time if accelerated by AI. While the Hub primarily focusses on AI-driven building lifecycle management, the cross-disciplinary team of Civil, AI, Manufacturing, Mechanical and Aeronautical engineering academics will facilitate seamless adoption of developed AI tools to aircraft lifecycle management, a key strategic priority of the UK Government in terms of technology leadership and achieving net-zero targets. The Hub will seek further long-term cross-disciplinary interaction with research groups working on ML and statistics, human behaviour within psychology and humanities and earth environment disciplines.

Grant Reference Number: EP/Y007786/1

Title: AI for Productive Research & Innovation in eLectronics (APRIL)

Team:

- Professor Themis Prodromakis, University of Edinburgh (PI)
- Dr Jacqueline Cole, University of Cambridge
- Dr Radu Sporea, University of Surrey
- Professor Dame Wendy Hall, University of Southampton
- Professor Kerstin Eder, University of Bristol
- Professor Máire O'Neill, Queen’s University of Belfast

Brief description of proposed work:

Artificial intelligence (AI) is undergoing an era of explosive growth. With increasingly capable AI agents such as chatGPT, AlphaFold, Gato and DALL-E capturing the public imagination, the potential impact of AI on modern society is becoming ever clearer for all to see. APRIL is a project that seeks to bring the benefits of AI to the electronics industry of the UK. Specifically, we aspire developing AI tools for cutting development times for everything from new, fundamental materials for electronic devices to complicated microchip designs and system architectures, leading to faster, cheaper, greener and overall more power-efficient electronics.

Imagine a future where extremely complex and intricate material structures, far more complex than what a human could design alone, are optimised by powerful algorithms (such as an AlphaFold for semiconductor materials). Or consider intelligent machines with domain-specialist knowledge (think of a Gato-like system trained on exactly the right milieu of skills) experimenting day and night with manufacturing techniques in order to build the perfect electronic components. Or yet what if we had algorithms trained to design circuits by interacting with an engineer in natural language (like a chatGPT with specialist knowledge)? Similar comments could be made about systems that would take care of the most tedious bits of testing and verifying increasingly complex systems such as mobile phone chipsets or aircraft avionics software, or indeed for modelling and simulating electronics (both potentially achievable by using semi-automated AI coders such as Google's "PaLM" model). This is precisely the cocktail of technologies that APRIL seeks to develop.

In this future, AI - with its capabilities of finding relevant information, performing simple tasks when instructed to do so and its incredible speed - would operate under the supervision of experienced engineers for assisting them in creating electronics suited to an ever-increasing palette of requirements, from low-power systems to chips manufactured to be recyclable to ultra-secure systems for handling the most sensitive and private data. To achieve this, APRIL brings together a large consortium of universities, industry and government bodies, working together to develop: i) the new technologies of the future, ii) the tools that will make these technologies a reality and very importantly, iii) the people with the necessary skills (for building as well as using such new tools) to ensure that the UK remains a capable and technologically advanced player in the global electronics industry.

Grant Reference Number: EP/Y007808/1

Title: Open Network for Artificial Chemical Intelligence & Discovery Hub (ON-ACID)

Team:

- Professor Leroy Cronin, University of Glasgow (PI)
- Dr Stephen Hilton, University College London
- Professor Benjamin Davis, University of Oxford
- Professor Jonathan Reid, University of Bristol
- Professor Oren Scherman, University of Cambridge
- Professor Richard Winpenny, The University of Manchester

Brief description of proposed work:

In chemistry and materials science the use of artificial intelligence (AI) approaches and machine learning (ML) is limited because the processes of data creation remain either analogue or non-standardised. The lack of a standard and specification for experiment set up means that data collection lacks context, and inference is not possible. If there is no executable ontology for chemical and materials discovery and synthesis then ML and AI methods cannot be applied to the sparse, error-ridden, and incomplete datasets. This deficiency was overcome in molecular biology as the developed ontology that linked protein sequence, synthesis, and structure enabled state-of-the-art ML systems like Alpha-fold to make vast progress in protein structure prediction.

Recently researchers in the UK, US, Canada, and Korea developed the concept of Chemputation, which established the abstraction of synthesis and discovery, via a programming language for chemistry / materials (XDL), and defined the hardware needed for execution and validation. This is vital for programming, automating, and the gathering of meaningful in-context chemical data, without which AI approaches cannot yield valuable results. Chemputation is the process of turning a program into an experiment to produce a given output - a new molecule, material, or experimental process.

In the ACID-hub we aim to build this infrastructure for chemistry and materials science by establishing universal, appropriate, and defined open standards for chemical and materials discovery and synthesis. By developing this standard, we will enable others to use the XDL programming language to design and run experiments, both manually and robotically, to produce reliable outcomes that can be digitally shared. ACID combines researchers from chemistry, robotics, sensing, computer science and interfaces with the key digital chemistry, biology, materials, chemical physics, and pharmacy centres across the UK, as well as academic, industrial and non-profits. Major improvements in reproducibility, gathering big data, discovery, and routes to efficient digital manufacture of materials and molecules will connect all the stake holders making the UK the place where the programmable matter revolution is born.

Grant Reference Number: EP/Y007875/1

Title: ML4Science: The AI Hub on Machine Learning for Science

Team:

- Professor Samuel Kaski, The University of Manchester (PI)
- Dr Anna Scaife, The University of Manchester
- Dr Carl Ek, University of Cambridge
- Dr Theodoros Damoulas, University of Warwick
- Professor Andrew Howes, University of Birmingham
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Brief description of proposed work:

Research is our most general and powerful method for finding solutions to problems, and new scientific knowledge and engineering innovations are urgently needed for improving productivity and addressing societal challenges. Yet, research practices and laboratories have largely remained unchanged, even though individual research tools have evolved. This hub will form an interface between AI methods and science and engineering, via virtual (simulation-based) laboratories, which will inspire and drive the development of transformative new machine learning methods. We seek to transform individual fields with novel methods, starting with research problems of our 4 core partners in engineering biology, engineering, materials and astronomy. Even more importantly, a bigger impact is expected to come from designing the virtual laboratories such that new tools can be more easily taken to use in new fields. This brings scale advantages when the methods are applied across multiple fields of science and engineering. An example is the so-called design-build-test-learn cycles driving engineering biology designs, which we will optimise for sustainable bioproduction and advanced therapeutics in Engineering Biology. The same techniques can be applied to optimise the use of large-scale facilities in Astronomy, significantly decreasing research costs, or for optimising traffic interventions for decreasing pollution. An ultimate goal is to generalise the technique to widely applicable discovery tools which combine collaborative AI approaches with machine learning based optimisation. Starting with the problems of our 4 core partners, demonstrating that methods can be applied across these seemingly very different fields, we will then extend the hub to other fields of science and engineering, and further to decision making in complex systems, for instance in healthcare, for which the general machine learning methods and the virtual laboratories concept are even more widely applicable.

The AI Hub ML4Science consists of leading researchers in four AI and Machine Learning themes needed for delivering this vision, working together with researchers of other disciplines to co-create use cases needing transformative solutions, and formulating the machine learning solutions. Participation of researchers in each of the other disciplines is coordinated by a leading researcher of the field, forming a "spoke" of the hub. Furthermore, we will engage with international networks of excellence for collaboration, and national and regional initiatives to bring new solutions forward with both existing industry and by incubating new startups.

Grant Reference Number: EP/Y00793X/1

Title: The National Hub for EMBodiED AI in Healthcare (EMBED-AI)

Team:

- Professor Praminda Caleb-Solly, University of Nottingham (PI)
- Dr Ayse Kucukyilmaz, University of Nottingham
- Professor Samia Nefti-Meziani, University of Birmingham
- Professor Duc Pham, University of Birmingham
- Professor Sanja Dogramadzi, University of Sheffield
- Professor Tony Prescott, University of Sheffield

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Brief description of proposed work:

The EMBED-AI hub will foster the co-development and validation of Embodied AI technologies, generating new paradigms for people and intelligent systems to interact intuitively and safely, also ensuring that sustainable and acceptable solutions are developed within a responsible research and innovation framework, as this is of paramount importance for any future deployment.

As noted in the recent BEIS research report (2021/043) Robotics and Autonomous Systems (RAS) have the potential to bring about significant economic impact with the annual global economic impact of advanced robotics estimated to lie between $1.7 to $4.5 trillion per annum by 2025, with potential for an extra $4.9 trillion per year to the global economy by 2030 by increasing installations. However, as they stand, RAS require significant advances if they are to make an impact in healthcare. Creative and innovate use of AI offers a solution. The UK still has an opportunity to locate itself as a leader in Embodied AI for Healthcare by addressing the fundamental research challenges for successful deployment in the real world. These include ensuring operational safety and efficacy required at multiple levels, which constitute key scientific challenges: effective situational awareness in unstructured human spaces, adaptive cognitive and physical human-robot interaction, shared control between humans and EAI systems, safe real-time failure management, and new circular and sustainable manufacturing design processes.

Ensuring reliability of such complex systems in the presence of multiple human users with different levels of physical, sensory and cognitive demands, within unstructured real-world environments, requires proficient and creative development and application of AI, integrating multidisciplinary approaches and end-user involvement from early stages. A complex plethora of safety concerns for Embodied AI Technologies create legal and regulatory issues, as well as raising concerns around trust and acceptability. The latter are compounded by issues resulting from economic uncertainty and fear of loss of jobs and lack of support in periods of rapid change.

Trust comes from transparency of system operation and decision-making processes, however for a system that adapts to changing environment and user needs, robust processes are needed to accurately communicate rationale for decisions and collaboratively test the validity of new behaviours.

Conversely, diverse embodiments present unique challenges for advancing AI. The opportunities afforded by embodied entities to physically sense and interact with the real-world, brings us closer to achieving more contextually intelligent interventions, better suited to augmenting our physical and cognitive limitations.

There is also a need to consider the wider implications of the roles people will play in co-designing and working alongside EAI technologies. There are issues relating to trust, user acceptance, ensuring human autonomy and dignity, skills development or re-skilling, and ensuring maximising human ingenuity and creativity in the face of automation. UKRI have initiated the creation of a landscape map which provides links to a wide range of UK innovators developing robotics, AI and key component technologies.

There are still poorly understood issues around commissioning, testing, installation and training requirements. These aspects, together with insurance and regulatory hurdles, are big barriers to deployment and adoption of Embodied AI technologies. The hub will bring together engineers and designers with relevant domain experts to address these barriers.

The Hub will work with industrial robot manufacturers in healthcare, also creating new innovation opportunities for low-cost design and manufacturing, to cross-fertilise ideas across domains, with a focus on selected use-cases in domestic service, healthcare monitoring, physical assistance, mobility and rehabilitation to advance AI.